

4-(4-hydroxybenzoyl)thiophene-2-sulfonamide

Inchi:	InChI=1S/C11H9NO4S2/c12-18(15,16)10-5-8(6-17-10)11(14)7-1-3-9(13)4-2-7/h1-6,13H,
InchiKey:	OJXOXNIZNJIMLU-UHFFFAOYSA-N
Formula:	C11H9NO4S2
SMILES:	NS(=O)(=O)c1cc(C(=O)c2ccc(O)cc2)cs1
Mol. weight [g/mol]:	283.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.86		Aqueous Solubility Prediction Method
logp	1.332		Crippen Method
mcvol	184.490	ml/mol	McGowan Method
tf	465.65	K	Aqueous Solubility Prediction Method

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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